Numerics of Partial Differential Equations

A portion of the applied mathematics research in the Mathematics and Computer Science Division at Argonne National Laboratory

Mission

- Provide solid mathematical foundations for the use of PDEs in applications of interest to the Of£ce of Science in the Department of Energy (DOE).
  - Algorithms
  - Software
  - PDE models
  - Tools for their analysis

Resources

- Principal Investigators
  - Gary Leaf (1 FTE)
  - Lois Curfman McInnes (.38 FTE)
  - Mike Minkoff (.3 FTE)
  - Barry Smith (.5 FTE)
- Postdoctoral Scholars
  - Mathew Knepley (.3 FTE)
- Investigators
  - Hong Zhang

Resources

- Technical Staff
  - Satish Balay (.5 FTE)
- Visiting Faculty
  - Padma Raghavan (Penn State University)
  - Jose Román (Polytechnic University of Valencia)
  - Juan Restrepo (University of Arizona)
- Students
  - Sanjukta Bhowmick (Penn State University)
  - Paulo Goldfeld (Courant Institute, New York University)
  - Dmitry Karpeyev (Old Dominion University)
  - Ernesto Prudencio (University of Colorado at Boulder)
  - Oliver Rheinbach (University of Essen, Germany)

Leverage (Our other funded work)

- SciDAC TOPS
- chem
- CCA ...

nteraction with Other Division Work

- Applied Mathematics
  - Computation of derivatives (automatic differentiation)
  - optimization
  - computational ¤uid dynamics
- MPI

In¤uence

- Biology
  - something
- Nano
  - something
- Algorithm research
  - something

Approach

- Identify the needs of important DOE applications,
- determine/develop the mathematics needed,
- design algorithms for high-performance computers based on the best (or most practical) mathematics,
- provide high-quality implementations of those algorithms usable by others.

For each of our projects (introduced below) we will step through these aspects of our work.

Technical Areas

Chapter 1: Algorithms and Software

- Implicit Solvers for Nonlinear PDEs
  - Mathematical Aspects of Multigrid Methods
  - Adaptive Polyalgorithmic Solvers
- Eigenvalue Computations for Computational Chemistry
  - SPAM – DFTB – SLEPc
- Automatic Generation of Discretizations and Error Estimators

Chapter 2: Modeling and Applications

- Dynamics of Micromagnetics
- Evolution of Structure in Interacting Particles
- Dynamic Systems and Computational Biology

Implicit Solvers for Nonlinear PDEs

- Taking advantage of the roots of the problem
  - multiple similar solves that arise sequentially
  - linear solve embedded in nonlinear problem
  - future work: in the context of moving meshes (below)

n Newton-Multigrid to Multigrid-Newton

$$F(u) = 0$$

Simple Newton's method may be written as

$$u \leftarrow u - J^{-1}(u)F(u).$$

Let $\bar{u}$ denote u with all components frozen at the beginning of the Newton step. Now Newton-SOR

$$u_i \leftarrow u_i - J_{ii}^{-1}(\bar{u})[F_i(\bar{u}) - \sum_{j=0}^{j<i} J_{ij}(\bar{u})(\bar{u}_j - u_j)].$$

SOR-Newton

$$u_i \leftarrow u_i - J_{ii}^{-1}(u)F_i(u).$$

Dynamics of Complex Systems

- Nanoscale properties of materials
  - Microstructure effects
  - Magnetic switching
  - Particle self-assembly
- Computational cell biology
  - Oscillations in metabolic networks
  - Cell population dynamics

Supporting Software and Algorithms

- Computational Material Science
  - Long-range £eld calculation
  - Conservative ODE/PDE discretizations
- Computational Cell Biology
  - Metabolic reconstruction
  - Parallel simulation of population dynamics

Material Microstructure Effects

- Implications to device performance, manufacturing
- Domain wall pinning in disordered magnetic composits
  - Elastic membrane in random pinning potential
  - Driven by *subcritical* applied force $F < F_c$
  - Critical slowing-down rate, £nal state roughness
  - Pinning preventing ergodic methods
- Large-scale numerical simulation and statistical sampling of potential
  - Three regimes in £nal approach
  - Determined critical exponent, symmetry $F < F_c < F$
- Collaboration with *MSD Theory Group*

aterial Microstructure Effects (cont'd)

- Vortex dynamics in type-II superconductors with random defects
  - SC states are minima of Ginzburg-Landau energy
  - Attained by GL gradient ¤ow preserving guage-invariance (Time-dependent GL)

$$\begin{aligned}\frac{\hbar}{2m_s D}\left(\frac{\partial}{\partial t}+\frac{ie_s}{\hbar}\Phi\right)\psi &= -\frac{1}{2m_s}\left(\frac{\hbar}{i}\nabla-\frac{e_s}{c}\mathbf{A}\right)^2\psi+a\psi-b|\psi|^2\psi,\\ \nu\left(\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}+\nabla\Phi\right) &= -\frac{c}{4\pi}\nabla\times\nabla\times\mathbf{A}+\mathbf{J}.\end{aligned}$$

  - Very long equilibration times due to phase transition
- Parallel integration of TDGL via domain decomposition
  - Family of scalable guage-invariant discretizations
  - Capture vortex creation and motion mechanism
  - *No* assumptions on vortex number, nature of

Magnetic Switching

- Coherent switching by coercive £eld H_a in granular disordered composits
  - Composition-controlled hysteretic properties
  - Improved Energy ef£ciency of magnet-based devices
  - Thermally assisted at critical $H_a >> 0$, timescale $\sim \mathsf{nsec}$
  - Hysteresis studies: consequtive equilibration runs at varied H_a
- Magnetic state decay
  - Thermally activated, $H_a \cong 0$
  - Incoherent, effected by *normal spin modes*
  - Timescale $\sim 1\mathsf{sec}$

Magnetic Spin Dynamics

- Landau-Lifshitz-Gilbert equation of motion

$$\frac{\partial \mathbf{M}}{\partial t} = \mathbf{M} \times \frac{\delta \mathcal{H}}{\delta \mathbf{M}} + \gamma \mathbf{M} \times \left(\mathbf{M} \times \frac{\delta \mathcal{H}}{\delta \mathbf{M}} \right),$$

$$\mathcal{H} = \int_{\mathcal{D}} d\S \left(A |\nabla \mathbf{M}|^2 + K |\mathbf{e} \times \mathbf{M}|^2 + \mathbf{H}_a \cdot \mathbf{M} \right) + \underbrace{\int_{\mathcal{D}} d\S \int_{\mathcal{D}} d\S' \left(\frac{\nabla \mathbf{M}(\S) \cdot \nabla \mathbf{M}(\S')}{|\S - \S'|} \right)}_{\mathcal{H}_{ff}}$$

- Spin length preservation $|\mathbf{M}| = const.$
- Global dipolar energy component $\mathcal{H}_{ff}$

Analysis and Numerics of LLG

- Issues
  - Stability and spin-length conservation
  - Invariants preservation (energy, undamped case)
  - Dipolar £eld solver performance
- Spin-length preserving integrator
  - Precession + damping decomposition
  - Improved stability
- Fast far £eld solver
  - Scalar potential+BI+multipole kernel expansion
  - Improved run-time, storage performance
- Local Lagrangian form of undamped local part

Switching Studies

- 1D spring-magnetic hysteresis
- Normal switching modes of iron nanodots

Notes for authors

Suggest having more info on slides that is printed only to notes version.
This could contain who is working on the material on that slide, and if it is background, past work or future work.

Ingedients for a PDE Simulation

- Governing weak form
  - Using Symbolic Expression components
- Domain geometry
  - Mesh component
- Discretization
  - Also Symbolic Expressions
- Boundary conditions
  - Also Symbolic Expressions

Component Veri£cation

- Necessary for Application “buy-in”
  - All results must come with con£dence bounds
- PDE need *a posteriori* error estimates
  - Generic framework is well-known

Code Generation for PDE

- Integration routines
  - Generated using geometry and basis function expressions
  - Leverage AD for Jacobians and Hessians
- Operator Assembly
  - Bookeeping needs mesh, unknown distribution on each element, and boundary conditions
- Boundary condition application
  - Code can be generated from the condition expressions
  - This also permits use of AD for sensitivites

Error Estimation Framework

- Solve the dual problem for a generalized Green function
  - Dual can be represented symbolically, exactly as the primal problem
  - This is also necessary for linear sensitivies
- Adaptivity
  - Control the error through mesh adaptation
  - Control constraint satisfaction or other error functionals

Proof of Concept

- Prototype Poisson and Bratu examples
  - All equations represented symbolically as ASTs
  - AST manipulation through the Visitor pattern
    - differentiation
    - variation
    - integration
    - interpretation or code generation
  - Dual-based error estimation
  - Mesh adaptation

Poisson Example I

$$
\begin{aligned}
-\Delta u &= f \text{ in } \Omega \\
u &= 0 \text{ on } \partial\Omega
\end{aligned}
\tag{1}
$$

u The solution

u_h The discrete solution from the space S

e The error $u - u_h$

z The dual solution, or generalized Green function

z_h The discrete dual solution

$$
\begin{aligned}
\langle \nabla z_h, \nabla \chi \rangle &= \langle e, \chi \rangle \text{ in } \Omega \\
\langle \nabla z_h, \nabla \chi \rangle &= 0 \text{ on } \partial\Omega
\end{aligned}
\tag{2}
$$

Poisson Example II

- The error is orthogonal to all elements χ of the test space

$$\begin{aligned} \langle \nabla e, \nabla \chi \rangle &= \langle \nabla (u - u_h), \nabla \chi \rangle \\ &= \langle f, \chi \rangle - \langle \nabla u_h, \nabla \chi \rangle \\ &= 0 \end{aligned} \tag{3}$$

- The error norm can then be written as

$$\begin{aligned} \|e\|^2 &= \langle e, e \rangle \\ &= \langle e, -\Delta z \rangle \\ &= \langle \nabla e, \nabla z \rangle \\ &= \langle \nabla e, \nabla (z - \chi) \rangle \, . \end{aligned} \tag{4}$$

Poisson Example III

- We may integrate element-wise, integrating by parts to obtain

$$\|e\|^2 = \sum_{\tau \in T_h} \left\{ \langle f + \Delta u_h, z - \chi \rangle_\tau - \frac{1}{2} \langle [n \cdot \nabla u_h], z - \chi \rangle_{\partial\tau} \right\}, \tag{5}$$

- The error has thus been split into two parts:
  - The equation residual
  - The ¤ux residual
- Each term is multiplied by the weighting function $z - \chi$
  - The dual solution gives a measure of the “in¤uence” of a given residual

Poisson Example IV

- Two obvious choices for the weighting function
  - $z_{h^+} - P_S z_{h^+}$, where S^+ is a richer space than S, and P_S the projector onto S
    - It is suf£cient for S' to be one polynomial order greater for P_k
  - $i_h^+ z_h - z_h$, where $i_h^+ z_h$ is an interpolant to H^+
    - This approach lacks mathematical foundation, but is much less expensive
    - Rannacher, et.al. report good experience on a number of practical problems
- For general linear functionals, we use the Reisz representation $J(e) = \langle e, \psi \rangle$

Missing Pieces

- Generation of language-speci£c expression graphs, and £nally code
- Enhanced discretization support
  - Advanced discretizations (spectral, discontinuous Galerkin)
  - Mixed discetizations
  - Multiple £elds
- Enhanced error estimation
  - Time-dependent problems
  - Hyperbolic problems

Biological Applications

- Mesh can represent a Metabolic Network
  - Automatic construction of ODE representation
  - Use AD seamlessly
- Incorporation of multi-parameter continuation

Optimization Applications

- Expressions for Variational Inequalities
  - Should only require *min* operation
- Support for PDE-constrained Optimzation
  - Leverage Veltisto

Geodynamics Applications

- 3D subduction
  - Allows investigation of large-scale patterns in volcanism
- Introduction of £nite elements
  - Allows error estimation and adaptation in troublesome corner region
- Multigrid and mesh re£nement for strongly variable viscosity
- Coupling with melting and reactive porous ¤ow
  - Likely to start with loose model coupling

Prior Work on Interacting Particles

- Participated in NSF Grand Challenge Simulation of Solid-Liquid Flow
  - Worked closely with Dan Joseph at University of Minnesota
  - http://www.e¤uids.com/e¤uids/books/joseph.html
- PETSc was used to simulate thousands of particles in ¤uid
- DNS on a moving, unstructured grid
- Scalable, multilevel preconditioning
- 85% parallel ef£ciency on 128 processors

Techiques for Particulate Flow

- Fictitious Domain Method
  - Could use an unstructured background mesh
    - Useful for strongly varying accuracy requirements
    - Can be adapted based upon error estimates
- Error Estimation
  - Constraint violation by FDM can be monitored
    - Use the constraint as the error functional J
    - Can control this error using adaptation of both meshes

Potential Reformulations

- Elastic bodies
  - Make use of *distributed* Lagrange multipliers
  - More general stress tensors are easily incorporated
- Implicit particle positions
  - Elegant resolution of the contact problem
  - Much more ef£cient than a moving mesh

SPAM

- Subspace Projection Approximation Method
- Extension of Davidson's Method to multilevel subspace approximations
- Designed for problems with expensive matrix vector costs
  - Hamiltonian matrices in Con£guration Interaction (CI), self-consistent £eld, molecular vibration analysis, cumulative reaction probability, and other areas of electronic structure calculations
- Uses a sequence of approximating matrices and generates expansion vectors at each approximating level

SPAM Cont'd

- Total number of matrix-vector calculations *may* increase, but numbe r of *true* matrix-vector evaluations will decrease
- Over 100 downloads from our FTP site

CRP (Application)

- Calculation of time-independent Cumulative Reaction Probability (CRP) to obtain exact reaction rates for large degree of freedom (DOF) problems
- Transition state theory (TST) rate constants effectively approximate CRP
  - Rarely calculated for more than 3 DOF, we seek to calculate 10 DOF
  - We can calibrate TST results by developing large-scale methods for CRP simulation and thus test widely used TST reaction rates coef£cients

CRP Approach

- Uses Lanczos method with each iteration requiring two inverse Green's functions evalutions
  - Inner iterations lead to solving a linear system for each Green's function
  - Solved via GMRES in PETSc
- Preconditioners
  - A sequential code has demonstrated that for some DOF, a truncated approximation of the banded matrix can obtain ef£cient GMRES convergence
  - In parallel, with diagonal preconditioning, problems of up to 7 DOF have been treated on 128 processors

CRP Preconditioning

- Discrete variable representation (DVR) leads to a sparse matrix
- Compared to £nite-difference matrices these matrices are
  - Smaller, but less sparse
  - More ill-conditioned
  - Higher values of Solver Iterations/Matrix dimension
- Collaboration with W. Poirier (DOE Early Career Award, Texas Tech University) on development of parallel optimal separable bases based upon block jacobi Factorization